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DUNDEE BIENNIAL CONFERENCE ON NUMERICAL ANALYSIS

UNIVERSITY OF DUNDEE

23 - 26 JUNE, 1987

ABSTRACTS

Section A Invited talks

Section B Submitted talks

US ARMY RESEARCH, DEVELOPMENT & STANDARDIZATION GROUP (UK)
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SECTION A

<u>The h-p Version of the Finite Element Method. Theory, Numerics and Industrial Experience</u>

I Babuska, University of Maryland, U.S.A.

The talk will present the basic, recent results of the h-p version of the finite element method and the applications. Numerical examples will be presented.

<u>The Numerical Solution of Initial-value Problems for Integro-Differential Equations</u>

H Brunner, Memorial University of Newfoundland, Canada.

In this talk we present a survey of recent developments in the numerical treatment of various types of Volterra integro-differential equations of order $r \geq 1$, including equations where the r-th derivative of the unknown solution occurs also in the kernel of the integral operator. The discussion will focus on theoretical and numerical aspects of spline collocation methods and on a related class of implicit Runge-Kutta-Nyström methods.

The talk will conclude with a look at some ongoing work regarding the numerical solution of partial Volterra integro-differential equations of parabolic and hyperbolic type.

<u>The Numerical Solution of Nonlinear Two-Point Boundary Value Problems using Iterated Deferred Corrections</u>

J R Cash, Imperial College, London.

Two of the most popular 'global' methods for solving general nonlinear two-point boundary value problems are collocation and deferred correction. For first order systems there is a well known equivalence between certain collocation and Runge-Kutta methods. In this talk we examine a method which combines these two approaches namely Runge-Kutta formulae with deferred corrections. In order to perform the deferred correction stage efficiently, a special class of formulae, known as Mono-Implicit Runge-Kutta formulae, is derived. The results of some extensive numerical computations, particularly for singular perturbation and turning point problems, are described.

Analysis and Computation for a Model for Possible Contamination by Nuclear Waste-Disposal in Porous Media

R E Ewing, University of Wyoming, U.S.A.

The transport through porous media of contamination generated by nuclear waste-disposal can be modelled by a system of four coupled nonlinear partial differential equations. The total fluid flow is described via an elliptic equation heat transport by a parabolic equation, and the miscible displacement of the dominant- and trace-species by transport-dominated parabolic equations. Since the fluid pressure appears in the three parabolic equations only through its velocity field, a mixed finite element method is used to approximate the fluid velocity directly. The heat, brine, and radionuclide are approximated via standard Galerkin procedures. Time stepping can be accomplished via implicit finite difference or modified method of characteristics techniques for the transport-dominated equations. Optimal order error estimates are derived when the imposed external flows are smoothly distributed. Concepts of adaptive local grid refinements are also discussed.

When things go wrong...

P W Gaffney, IBM, Norway.

This talk is a personal account of my observations on the state of mathematical software and what I believe numerical analysts must do in order to influence computer users to use good numerical techniques.

Inexact Solutions and Domain Decomposition

G H Golub, Stanford University, U.S.A.

In many situations, domain decomposition is equivalent to partitioning a matrix into submatrices and then solving a system of equations associated with each submatrix. Unfortunately, it is not possible to solve each subsystem exactly. An inner-outer iteration procedure is necessary in obtaining the approximate solution on the subdomain. In this talk, we analyse the Chebyshev semi-iterative method for matrices that possess "Property A" and show the convergence properties of the algorithm.

On the Dynamics of Certain Time Integrators with Step-size Control

D F Griffiths, University of Dundee.

When evaluating some low order predictor-corrector methods with step-size control for possible use in time dependent PDES, an extremely erratic behaviour was encountered as the solution approached its asymptotic state. This behaviour could not, in general, be alleviated by adding constraints such as imposing a bound on the ratio of consecutive time steps.

In this talk we shall investigate the causes of such phenomena in very simple situations and analyse certain schemes both from the point of view of dynamical systems and by the use of modified equations.

Some New Classes of Mixed Finite Element Methods

T J R Hughes, Stanford University, U.S.A.

We describe two general classes of mixed finite element methods which possess better stability properties than the classical Galerkin formulation. The first class enables convergence theorems to be established while circumventing entirely the Babuška-Brezzi condition. Methods of this type (termed "CBB methods") have been developed which permit a wide variety of convergent interpolations, many of which are unstable in the Galerkin formulation. For example, a CBB formulation of the Stokes problem is described which is convergent for all combinations of continuous velocity and continuous or discontinuous pressure interpolations. The second class of methods permits satisfaction of the Babuška-Brezzi condition and a-ellipticity condition for a much wider class of interpolations than the Galerkin method ("SBB methods"). Applications to problems arising in structural mechanics are described.

Order Barriers for Difference Schemes for Linear and Nonlinear Hyperbolic Problems

R Jeltsch, RWTH Aachen, Germany.

For the constant coefficient advection equation, starting from known results for one-step schemes, we conjecture the existence of an order Courant-Friedrichs-Lewy condition for multistep methods. Partial results supporting this conjecture are given. In the nonlinear part of the paper we concentrate on one-step schemes for a scalar hyperbolic conservation law. The order conditions are given and the order of the Random-Choice method is investigated. Old and new order barriers due to different properties of the schemes are presented.

Arithmetic for Vector Processors
U Kulisch, University of Karlsruhe, Germany.

In electronic computers the elementary arithmetic operations are these days generally approximated by floating-point operations of highest accuracy. *Computer arithmetic, however,* can be extended so that the arithmetic operations in the linear spaces and their interval correspondents which are most commonly used in computation can be performed with highest accuracy on digital computers also. The basic building blocks of these additional arithmetic operations are discussed.

In recent years there has been a significant shift of numerical computation from general purpose computers towards vector and parallel computers - socalled supercomputers. Besides the elementary arithmetic operations +, -, *, /, supercomputers usually offer a number of compound operations as additional elementary operations. Such elementary compound operations are for example: "multiply and add", "accumulate" or "multiply and accumulate". Also these operations shall always deliver an answer of highest accuracy whatever the data are. Diverse methods are discussed which allow a fast and correct computation of elementary compound operations as well as all basic operations for extended computer arithmetic. Pipeline techniques are used to obtain high speed for these operations. In a scalar product computation these methods allow the execution of a multiplication and the corresponding addition in each cycle time.

The methods discussed in the paper can also be used to build a fast unit for advanced arithmetic for micro computers in VLSI-technology.

Robust Non-linear Data Fitting
K Madsen, Technical University, Denmark.

During the last decades there has been much interest in replacing the least squares criterion in data fitting with a more "robust" criterion. One of these is Huber criterion where the smaller residuals are measured by the l_2-norm and the larger by the l_1-norm.

We give an introduction to the Huber criterion for data fitting. Algorithms for the linear case are reviewed, and a new trust region method for the nonlinear case is presented. The latter method is illustrated through numerical examples.

Subdivision and Refinement Algorithms for Curves and Surfaces
C Micchelli, IBM, New York.

We will survey some subdivision techniques used in computer aided design for the computation of curves and surfaces and also report on recent joint work with H. Prautsch.

Multivariable Approximation Using Radial Basis Functions

M J D Powell, University of Cambridge.

Our approximating functions have the form

$$s(x) = \sum_{i=1}^{m} \lambda_i \phi(\|x-x_i\|_2), \qquad x \in \mathbb{R}^n$$

where the $\{\lambda_i : i=1,2,\ldots,m\}$ are real coefficients, $\phi(.)$ is a fixed function from $\mathbb{R}^+$ to $\mathbb{R}$, and $\{x_i : i=1,2,\ldots,m\}$ is a set of prescribed points in $\mathbb{R}^n$. They seem to be highly useful for approximation to continuous functions from $\mathbb{R}^n$ to $\mathbb{R}$, because the points $\{x_i : i=1,2,\ldots,m\}$ can be made more dense where higher accuracy or more flexibility is required. We consider published work on choices of $\phi(.)$, interpolation on $\{x_i : i=1,2,\ldots,m\}$, basis functions for the linear space that is spanned by $\{\phi(\|x-x_i\|_2) : x \in \mathbb{R}^n\}$ $(i=1,2,\ldots,m)$, the addition of a low order polynomial to $s(.)$, and convergence properties. The cases $\phi(r)=r$ and $\phi(r)=r^3$ when $n=2$ are demonstrated by numerical examples.

Review of some Results on Modulational Instabilities in Nonlinear Difference Schemes

D M Sloan* and B M Herbst, University of Strathclyde.

The numerical solution of a nonlinear difference equation may become unstable in situations where the exact solution of the difference equation should remain bounded. Newell discussed this phenomenon and attributed it to a focusing mechanism which localises energy on the spatial grid. Here we review some results obtained using leap-frog discretisations of the advection equation and the KdV equation. Numerical results show a modulation of the envelope of the basic solution and, as this modulation takes place, there is a growth in Fourier modes in the vicinity of the fundamental mode. The solution evolves in time with variations which depend on more than one time scale. A multiple scales analysis is described which throws some light on the structure of the instability.

A Study of Rosenbrock Methods for Differential and Differential-Algebraic Problems

G Wanner, University of Geneva, Switzerland.

<u>Computational Methods for Bifurcation Problems with Symmetries and Applications to Steady States of n-box Reaction-diffusion Models</u>

B Werner, University of Hamburg, Germany.

We consider parametrized nonlinear equations (equilibrium problems)

(1.1) $$g(x,\lambda) = 0, \quad g: X \times \mathbb{R} \to X, \quad X = \mathbb{R}^n$$

satisfying a symmetry condition

(1.2) $$g(\gamma x,\lambda) = \gamma g(x,\lambda), \quad x \in X,\ \lambda \in \mathbb{R},\ \gamma \in \Gamma,$$

with a symmetry group $\Gamma \subset O(n)$. Discretized nonlinear boundary value problems with symmetric domain or symmetrically coupled n-box reaction-diffusion models lead to (1.1), (1.2).

Due to the symmetry, (1.1) can carry a rich bifurcation structure: there might be several Σ-branches of solutions of (1.1) having the symmetry of a subgroup Σ of Γ and being connected with other $\tilde{\Sigma}$-branches via Σ-$\tilde{\Sigma}$-(symmetry-) breaking (multiple) bifurcation points.

It is shown how group theoretical ideas and bifurcation results (Cicogna [1981], Vanderbauwhede [1982], Golubitsky - Stewart - Schaeffer [1987] *allow an efficient computation* of the solution diagram of (1.1), especially of the bifurcation points. The essential step is a reduction process corresponding to suitable isotropy subgroups Σ of Γ. Assuming irreducible representations of Γ on the kernel of a singular point of g, multiple bifurcation points are reduced to simple (e.g. pitchfork) bifurcation points and the extended system in Werner-Spence [1984] (treating the case of Z_2-symmetry) can be used for their computation. Numerical results for certain 4-box Brusselator models are given. Related aspects for the construction of Gaussian cubature rules for certain domains with symmetry are mentioned.

SECTION B

Some Practical Experience on a Parallel Computer

C A Addison*; J Petersen; R M Chamberlain, Chr. Michelsen Institute, Bergen, Norway.

We present an overview of the parallel computing activities at Chr. Michelsen Institute over the last year and a half. These include aspects of seismic processing, the solution of the 2D wave equation in inhomogeneous media and the solution of dense systems of linear equations. This presentation focuses on the latter two topics.

Certain operations among the nodes of the Hypercube are used frequently. A high level library of such operations is evolved in order to make using the Hypercube easier. It is intended that such a library hide machine dependencies from users, thus providing a common interface for an application of any Hypercube based architecture.

We conclude with a summary of what we have learned in these initial efforts of solving problems in parallel and provide an indication of what our future developments might be.

Experiments with the BFGS and DFP Updates on Various Positive Definite Matrices

M Al-Baali, University of Damascus, Syria.

In this talk we consider the possibility of correcting the current matrices, which approximate the Hessian matrix or its inverse, in certain sense, before updating either by the BFGS or by the DFP formulae. This approach leads to definite various classes of formulae for minimizing unconstrained problems, and one of them is the well known Broyden family of formulae. Numerical results are given to illustrate most cases.

A Comparison of One-Dimensional Solution Techniques Applied to the 2-D Euler Equations

J J Barley, University of Reading.

Approximate solutions of the two-dimensional Euler equations of compressible flow are often obtained by operator splitting where a one-dimensional difference operator is applied alternately in each coordinate direction. Alternatively, the simultaneous application of one dimensional difference operators in each direction may be used.

A comparison is presented between such techniques for two test problems (mild and severe) using both the flux-difference split scheme of Roe and the flux-vector split scheme of Steger-Warming. Results are illustrated graphically.

Natural Conti us Extensions of Runge-Kutta Methods for V erra Integral Equations of the Second Kind and their Applications

A Bellen; Z Jackiewicz; R Vermiglio*; M Zennaro, Universita' di Udine, Italy.

We consider a very general class of Runge-Kutta methods for the numerical solution of Volterra integral equations of the second kind, which includes as special cases all the most important methods which have been considered in the literature. The main purpose of this paper is to define and prove the existence of the Natural Continuous Extensions (NCEs) of Runge-Kutta methods, i.e. piecewise polynomial functions which extend the approximation at the grid points to the whole interval of integration. The particular properties required of the NCEs allow us to construct the tail approximations, which are quite efficient in terms of kernel evaluations and also result in good stability properties of the proposed numerical methods.

Global Error Estimation in the Method of Lines for Parabolic Equations

M Berzins, Leeds University.

A method is described for obtaining an indication of the error in the numerical solution of parabolic partial differential equations using the method of lines. The error indicator is derived by using a combination of existing global error estimating algorithms for initial value problems in ordinary differential equations, [1] with estimates for the p.d.e. truncation error which are obtained by using Richardson extrapolation. An implementation of the algorithm is described and numerical examples are used to illustrate the reliability of the error estimates that are obtained. The efficiency of the algorithm is evaluated and various different approaches compared. The application of the method to the design of reliable algorithms for partial differential equations is considered.

[1] L.F.Shampine: Global Error Estimation for Stiff O.D.E.s. Proc. of Dundee Conference on Numerical Analysis 1983, Springer Verlag Lecture Notes in Mathematics No 1066.

Numerical Methods for the Space Charge Equation

C Budd, Oxford University.

The space charge equation is a third order nonlinear PDE of mixed type which models the steady electrostatic field in a neighbourhood of a coronating electrode. By employing a hodograph transformation we may rewrite the equation as a coupled nonlinear elliptic equation and an ODE on a rectangular domain. This transformation leads to an effective numerical scheme based upon a finite difference approach, which can cope with a wide variety of geometries and boundary conditions for the original problem.

Convergence of Univariate Quasi-Interpolation Using Multiquadrics

M D Buhmann, University of Cambridge.

Univariate interpolation using the radial-basis-function $\phi: R \to R$ for an infinite number of equally-spaced real data-points of spacing $h > 0$ can be performed by choosing the element ψ of the linear space X spanned by $\{\phi(|\cdot-jh|) \mid j \in Z\}$ that satisfies $\psi(ih) = \delta_{i0}$ and defining the interpolant $s: R \to T$ to $f: R \to R$ by

$$s(x) = \sum_{j=-\infty}^{\infty} f(jh)\psi(x-jh), \quad x \in R,$$

which yields $s(ih) = f(ih) \ \forall\, i \in Z$.

Restricting ψ to a finite-dimensional subspace of X and giving up the condition $\psi(ih) = \delta_{i0}$, we consider quasi-interpolants $s: R \to R$ of the form given and study their convergence behaviour with regard to localization properties of ψ. If twice differentiable functions f with $|f(x)| = O(|x|)$ for $x \to \pm\infty$ are approximated and if Hardy's multiquadric formula $\phi(r) = \sqrt{r^2 + c^2}$ is chosen for $c > 0$, localization is sufficient to prove convergence of the approximation scheme as $h \to 0$. When $\phi(r) = 1/\sqrt{r^2 + c^2}$, however, as in the inverse multiquadrics formula, sufficient localization cannot be obtained.

Studying the influence of the choice of the parameter c in the multiquadrics formula on the quality of the approximation, we find that c/h has to remain bounded as $h \to 0$. Otherwise there are smooth and bounded functions for which the quasi-interpolants given do not converge to the said functions.

We finally give numerical examples that suggest that in the cases of multiquadrics and inverse multiquadrics where now again $\psi(ih) = \delta_{i0}$ and ψ is an element of the whole space X, good localization properties of ψ are achieved.

The Characteristic Galerkin Method for Nonlinear Hyperbolic Systems

P. Childs, Oxford University Computing Laboratory.

We describe the application of the characteristic Galerkin method to nonlinear systems of hyperbolic conservation laws, especially for shock modelling. For a scalar equation, the basic characteristic Galerkin scheme, based on piecewise constant elements is first order; adaptive recovery techniques give second order accuracy for smooth solutions. The method is extended to systems via flux-splitting. Our formulation easily allows the use of moving and adaptive grids. There is no stability restriction imposed on the timestep: choice of the grid and timestep can be made solely from considerations of accuracy. A full analysis for a scalar equation demonstrates several interesting features of the method. We illustrate the application to systems of equations through a series of one-dimensional test problems.

A Numerical S , of Nonlinear Waves in a Fluidized Bed

I Christie*; G Ganser, West Virginia University, U.S.A.

A third order nonlinear problem approximating the vertical flow in a one dimensional fluidized bed is solved by a Petrov-Galerkin method. Piecewise linear trial functions, cubic spline test functions and product approximation lead to a fourth order discretization in space. Second order backward differentiation is used for the time integration. Experiments show that while some values of the time step may produce stable results, a reduction in the time step introduces instability. This behaviour is confirmed by a von Neumann stability analysis of a simplified problem.

Numerical Methods for $y'' = f(x,y)$ via Rational Approximations for the Cosine

J P Coleman, University of Durham.

Many numerical methods, when applied to the scalar test equation $y'' = -\omega^2 y$, yield a three-term recurrence relation which has a characteristic equation of the form

$$\zeta^2 - 2R_{nm}(\nu^2)\zeta + 1 = 0;$$

here $\nu = \omega h$, where h is the steplength, and R_{nm} is a rational function. Examples include Runge-Kutta-Nyström methods [van der Houwen and Sommeijer (1987a)]. Numerov's method and several related hybrid methods "Chawla (1983, 1984), Chawla and Rao (1984, 1986)], and some other multistep methods [Cash (1981), Thomas (1984), van der Houwen and Sommeijer (1987b)].

The properties of $R_{nm}(\nu^2)$ as a rational approximant for $\cos\nu$ can be used to investigate the order of dispersion (phase-lag) and the stability of such methods. In particular:

(1) For given n and m, the degrees of numerator and denominator, the maximal order of dispersion is 2n + 2m, which is obtained when $R_{nm}(\nu^2)$ is the [2n/2m] Padé approximant for $\cos\nu$.

(2) For explicit methods of maximal order of dispersion $R_{nm}(\nu^2) = p_{2n}(\nu)$, the Maclaurin polynomial of degree 2n for $\cos\nu$. Any such method has an interval of periodicity $(0,\nu^2{}_n)$ where

$$\nu_1 < \nu_3 < \nu_5 < \ldots < \pi < \nu_2 < \nu_4 < \ldots < 2\pi.$$

(3) Methods corresponding to the [0/2m] Padé approximants for $\cos\nu$ are P-stable.

Calculat... of Solutions of some P.D.E. with Two- and ...reedimensional Singularities

L Collatz, University of Hamburg, Germany.

Inclusion theorems for solutions of some types of boundary value problems with singularities in R^2 and R^3. Improvement of the error bounds with aid of Bessel functions of not integer index.

Primal Methods are Better than Dual Methods for Solving Overdetermined Linear Systems in the l-infinity Sense

A R Conn; Yuying Li; R Bartels: University of Waterloo, Canada.

It is generally believed that methods based upon solving the dual of the linear programming formulation of the linear Chebychev problem are superior to methods based upon the primal formulation.

We present a primal approach along with evidence that for random problems primal methods are to be preferred. We then show that the method that is generally considered the best algorithm for discrete linear approximation in the l-infinity norm actually owes much of its efficiency to effective choice of a starting point. This phenomenon is explained with the aid of results from classical minimax theory, which is then used to determine a suitable initial point for a primal method.

With this enhancement it would appear that the primal approach is also preferable for data-fitting problems.

Implementation Schemes for Implicit Runge-Kutta Methods

G J Cooper, University of Sussex.

Iterative procedures, for the implementation of implicit methods applied to stiff problems, are considered. Some schemes, which are based on the use of projection methods, are obtained. These schemes avoid the need to solve systems of linear equations.

Least Squares ..rcle Fitting to Data with Specified Uncert..../ty Ellipses

M G Cox; H M Jones*, National Physical Laboratory.

We consider the problem of fitting a circle to a set of data points specified in terms of their Cartesian coordinates. We assume that the data adequately represents a circle and that associated with each point there is an uncertainty ellipse describing the measurement error. We formulate a weighted nonlinear least squares problem in order to determine unbiased estimates of the coordinates of the centre and the radius of the circle which best fits the data. The weights used in forming the objective function for this optimization are derived from the given ellipse parameters. The resulting problem displays structure which is exploited when the Gauss-Newton algorithm is used to obtain a solution. Initial values for the method are estimated from a linear approximation to the nonlinear fitting problem.

In addition to estimates of the circle parameters the algorithm produces their variance/covariance matrix from which an error ellipse for the centre of the circle may be deduced.

Problems involving circle fitting have arisen recently in two distinct areas of work at NPL - dimensional metrology and microwave measurement. A data set from one of these areas is used to illustrate the algorithm.

Stability of the Exact Collocation Method for the Second Kind Volterra Integral Equation with Degenerate Kernel

M R Crisci; E Russo; A Vecchio, University of Naples.

We analyze the stability properties of the exact collocation method applied to a second kind Volterra integral equation with degenerate kernel:

$$(1) \qquad y(t) = g(t) + \int_0^t \sum_{i=1}^{n} A_i(t)\, B_i(t) y(s) ds$$

The kernel of (1) is a generalization of polynomial convolution kernel, and it can be considered a significant test ternel, as the class of (1) is dense in the class of all continuous kernels $k(t,s)$.

We derive a recurrence formula for a vector containing the numerical solution in the collocation points, and we obtain stability conditions.

Moreover, for the known convolution test equation whose kernel

$$(2) \qquad k(t,s) = \lambda + \mu\,(t-s)$$

is a particular case of (1), we individualize, under the hypothesis that the collocation points are symmetric, the stability regions.

Data Smoothing by Divided Differences Using Least Squares Approximation

M P Cullinan, National Institute for Higher Education, Ireland.

The following technique is proposed for removing errors in n measurements $f_j(x_j)$, $1 \le j \le n$, of values of an underlying smooth function. Calculate the consecutive divided differences of a chosen order r of the data. If any of these divided differences are negative, find points y_j to minimise $\sum_{j=1}^{n} (f_j - y_j)^2$, where the y_j are subject to the constraints that their consecutive divided differences of order r be non-negative. When $r \ge 3$ the set of points so constrained is larger than might appear, and the calculations required by this method can be performed very quickly. The class of data amenable to this method is limited only by the extent that the underlying function undulates. Some undulation can be accommodated by increasing r.

An Effective and Simple Adaptive Mesh for Enthalpy Formulations of Multi-Phase Moving Boundary Problems

D B Duncan, Heriot-Watt University.

A method for moving the mesh in enthalpy formulations of multi-phase moving boundary problems is presented. The method is based on the equidistribution of a function which has constant value C_0 outside the phase change regions and takes values larger than C_0 in the transition region. This concentrates the mesh points in and near the phase change zones and leaves them equally spaced outside such regions. It works well on classical Stefan problems and on problems with mushy regions.

The method is based loosely on a technique described by Sanz-Serna and Christie (J. Comp. Phys. V67 p348, 1986), but uses a true moving mesh formulation instead of their interpolation method. The mesh distribution procedure is very simple to program and the PDE solver is standard.

Admissible Slopes for Monotone and Convex Interpolation

A Edelman*; C A Micchelli, MIT, U.S.A.

In many applications, interpolation of experimental data exhibiting some geometric property such as nonnegativity, monotonicity or convexity is unacceptable unless the interpolant reflects these characteristics. This paper identifies admissible slopes at data points of various C^1 interpolants which insure a desirable shape. We discuss this question, in turn for the following function classes commonly used for shape preserving interpolations: monotone polynomials , C^1 monotone piecewise polynomials, convex polynomials, parametric cubic curves and rational functions.

Automatic Imple. .ation of an Initial Value Method for use Two-Point Boundary Problems

R England*; R M Mattheij, Polytechnic of the South Bank.

Two-point boundary value problems often have sharp boundary layers, or rapidly varying fundamental modes. These make a uniform discretization inefficient, and iterative adaptive refinement may also be undesirable, particularly for linear problems. With a sequential marching approach, it should be possible to select reasonable step sizes in a single pass, based on numerical estimation of layers and of a smooth particular solution. Normal integrators for initial value problems select their step sizes on the basis of asymptotic error estimates for small step sizes. However, these may be large in the presence of fast growing fundamental modes, unless the step size is much smaller than necessary. In this talk, a new form of error indicator will be outlined, which enables an integrator to take an appreciable number of steps of a suitable size for such a problem, without generating excessively unstable solutions. After a starting-up stage, a special explicit predictor may be matched to an appropriate implicit corrector in such a way that their difference, while asymptotically correct for small step sizes, is also an appropriate error indicator for large step sizes. Efficient and stable iterative methods will also be discussed for solving the linked correction formulae which are used, while maintaining their stability properties. A few results will show the feasibility of finding smooth solutions with appropriate step sizes.

An Analysis of Defect-Control Strategies for Runge-Kutta Methods

W H Enright, University of Toronto, Canada.

Over the last three decades there has been a considerable change in what is expected of a general purpose Runge-Kutta method for initial value problems. Discrete, fixed-stepsize methods have been replaced by discrete, variable-step methods which attempt, with mixed success, to match the achieved accuracy with a tolerance parameter, TOL. Now, with the development of inexpensive interpolants, it is feasible to expect a Runge-Kutta method to produce a continuous solution approximation with an accuracy which is directly related to TOL. In this paper we analyse several error control-strategies which are designed to achieve this objective. We will present theoretical and experimental evidence to show that this approach is viable and can lead to a family of methods that are effective and much easier to use than existing methods.

Discrete-Time Finite Element Methods for Parabolic Integro-Differential Equations

G Fairweather*; E G Yanik, University of Kentucky, U.S.A.

In the modeling of some space-time dependent physical systems in such fields as heat transfer, nuclear reactor dynamics and viscoelasticity, it is often necessary to take into account memory effects. In the mathematical model of such a system, this results in the inclusion of an integral term in the basic differential equation yielding a partial-integro differential equation (PIDE). The equations considered in this paper are PIDEs of parabolic type of the form

$$(1) \quad u_t + \nabla(a(x,t,u)\nabla u) = \int_0^t f(x,t,s,u(x,s),\nabla u(x,s))ds, \qquad (x,t) \in \Omega \times (0,T],$$

where Ω is a bounded domain in R^n, $n=1,2$. While much attention has been paid in the recent literature to the study of various properties of solutions of problems of this kind, little has been reported on the development and analysis of numerical techniques. In this paper, we describe several discrete-time finite element procedures for the numerical solution of (1). Galerkin's method or spline collocation at Gauss points is used for the spatial discretization, and both nonlinear and algebraically linear time-stepping methods are discussed. Under certain conditions, the methods yield approximations which are second order accurate in time and of optimal accuracy in space. Similar methods for certain hyperbolic PIDEs are also described.

An Error Bound for Multivariate Lacunary Interpolation

T Fawzy, Suez-Canal University, Egypt.

In [1], we presented a method for solving the general lacunary interpolation problem, using polynomial splines, which gives optimal error bounds. In [2], we introduce a tensor version of our general method which can be used to solve lacunary interpolation problems in two or more variables.

The purpose of this paper is to obtain an optimal error bounds for a special case of the method described in [2].

[1] Th. Fawzy and L.L. Schumaker: A piecewise polynomial lacunary interpolation method. Journal of Approximation Theory, Vol.48, No.4, December 1986, pp.407-426.

[2] Th. Fawzy and L.L.Schumaker: Multivariate Lacunary Interpolation. Proceeding of the Fifth International Symposium on Approximation Theory held at Texas A & M University on January 13-17, 1986. Academic Press 1986, pp.339-342.

Nonlinear Programming and Nonsmooth Optimization by Successive Linear Programming

R Fletcher*; E Sainz de la Maza, University of Dundee.

Methods are considered for solving nonlinear programming problems using an exact ℓ_1 penalty function. LP-like subproblems incorporating a trust region constraint are solved successively both to estimate the active set and to provide a foundation for proving global convergence. In one particular method, second order information is represented by approximating the reduced Hessian matrix, and Coleman-Conn steps are taken. A criterion for accepting these steps is given which enables the superlinear convergence properties of the Coleman-Conn method to be retained whilst preserving global convergence and avoiding the Maratos effect. The methods generalize to solve a wide range of composite nonsmooth optimization problems and the theory is presented in this general setting. A range of numerical experiments on small test problems is described.

The Pseudospectral Method: Comparisons with Finite Differences for the Elastic Wave Equation

B Fornberg, Exxon Research, U.S.A.

The pseudospectral method is a technique for solving hyperbolic systems of equations. It is much less flexible than finite differences, for example with regard to boundaries and adaptive meshes. However, in applications where its limitations are not important, very large savings in computer time and storage may be achieved. Early applications include homogeneous turbulence, nonlinear waves and weather/climate modeling. In this presentation, we will first briefly review the background of the method and then illustrate its performance in the case of elastic waves propagating through two-dimensional discontinuous media.

Adaptive Grid Methods for Nonlinear Dispersive Wave Equations

E Fraga, University of Dundee.

Adaptive grid methods for nonlinear dispersive wave equations are discussed. Particular attention is placed on the Korteweg-de Vries and Nonlinear Schroedinger equations.

Pictures of Karmarkar's Linear Programming Algorithm

D M Gay, AT & T Bell Laboratories, U.S.A.

Karmarkar's linear programming algorithm handles inequality constraints by changing variables to make all constraints about equally distant; it moves in the steepest-descent direction seen by the new variables. This paper summarizes four variants of Karmarkar's linear programming algorithm (primal affine, primal projective, dual affine, and dual projective), discusses depicting polytopes (feasible regions), and presents pictures illustrating the latter three variants. These pictures give an algorithm's eye view of the variable changes and provide visual verification of certain properties.

On Approximate Solutions of One Class of Integral Equations

L Hacia, Technical University of Poznan, Poland.

Various methods of approximate solution for certain class of integral equations are presented. Sufficient conditions for the convergence of the considered methods are given and the error estimates are established.

The comparison is made among introduced methods, that are illustrated by examples.

A Multilevel Parallel Solver for Banded Linear Systems

I N Hajj; S Skelboe*, University of Copenhagen, Denmark.

The talk describes an algorithm for the parallel LU-factorization and solution of banded systems. For a system of dimension n with bandwidth $2m+1$, a parallel computer with $n/(2m)$ processors and suitable communication topology will be able to perform factorization and solution in $O(m^3 \log_2(n/m))$ time units. The hypercube topology is an example of a suitable communication topology. The speedup of the algorithm as compared to the direct solution using a single serial processor is $O((n/m)/\log_2(n/m))$.

The algorithm is based on a reordering strategy also known from nested dissection where a set of separator variables and equations are identified and ordered last to make the system appear as a set of connected sub-systems. The sub-systems are LU-factored in parallel leaving the separator equations partially factored with the structure of a block tridiagonal system. The dissection, reordering and parallel partial LU-factorization is applied to the block tridiagonal system and repeated until the system is completely factored. This part is closely related to cyclic reduction of a block tridiagonal matrix. However, the result of the proposed algorithm is identical to a standard LU-factorization applied after the reorderings.

The solution phase can also be done in parallel either after the completion of the LU-factorization or with the forward substitution pipelined immediately after the LU-factorization.

The proposed algorithm does not permit pivoting for numerical reasons but is otherwise rather flexible. It can be applied to any matrix with a block tridiagonal envelope which includes band matrices, and if the matrix is symmetric and positive definite, Cholesky's method can readily be substituted for the LU-factorization.

Numerical Simulation of Flow in Porous Media

D E Heath, University of Reading.

A production method for the extraction of heavy oil is to inject steam into the reservoir so as to lower the viscosity of the oil, thus allowing extraction by conventional means, the tracking of the steam front during the injection cycle being an important factor in optimizing the production.

In this talk a mathematical model for the simpler problem of injecting hot water into a porous medium is described and the resulting differential equations are solved by finite element methods.

On the Growth of Simplices in Nelder-Mead Simplex Reflections

D Hensley; P W Smith*; D J Woods, IMSL, U.S.A.

We derive relationships between the elements of a sequence of simplices, where each simplex in the sequence is produced by applying a simplex reflection operation to the previous element of the sequence. The reflection operation is one of four simplex operations used in the Nelder-Mead simplex algorithm for function minimization. The relationships derived here are of use in proving convergence properties of the Nelder-Mead algorithm.

On the Stability of Nonlinear Difference Schemes

B M Herbst, University of the Orange Free State, South Africa.

This talk looks into more detail at one of the situations described by D.M. Sloan. It is shown how nonlinear difference schemes may be destabilised through resonances between the different waves constituating the solution. The multiple scales analysis is described and numerical examples are given

Analysis of the Enright-Kamel Partitioning Method for Stiff ODEs

D J Higham, University of Manchester.

The use of implicit formulae in the solution of stiff ODEs gives rise to systems of nonlinear equations which are usually solved iteratively by a modified Newton scheme. The linear algebra costs associated with such schemes may form a substantial part of the overall cost of the solution. Enright and Kamel [7, 10] attempt to reduce the cost of the iteration by automatically transforming and partitioning the system. We provide new theoretical justification for this method in the case where the stiff eigenvalues of the Jacobian matrix used in the modified Newton iteration are small in number and well separated from the other eigenvalues. The theory of Saad [15, 16] is introduced and adapted to show that the method uses the projection of the Jacobian onto a Krylov subspace which virtually contains the dominant subspace. This is shown to have favourable consequences. Numerical evidence is provided to support the theory.

Fortran Codes for Estimating the One-norm of a Real or Complex Matrix, with Applications to Condition Estimation

N J Higham, University of Manchester.

Fortran 77 codes SONEST and CONEST are presented for estimating the 1-norm of a real or complex matrix respectively. The codes are of wide applicability in condition estimation since explicit access to the matrix, A, is not required; instead, matrix-vector products Ax and $A^T x$ are computed by the calling program via a reverse communication interface. The algorithms are based on a convex optimisation method for estimating the 1-norm of a real matrix devised by Hager [SIAM J. Sci. Stat. Comput. 5 (1984), pp.311-316]. We derive new results concerning the behaviour of Hager's method, extend it to complex matrices, and make algorithmic modifications in order to improve the reliability and efficiency.

Numerical Fixed Domain Mapping Solution of Free Surface Flows Coupled with an Evolving Interior Field

R C A Hindmarsh*; K Hutter, Edinburgh University.

The problem of a gravity-driven free-surface flow coupled with the evolution of an interior field is solved using a finite difference discretization of a mapping of the problem onto the unit square. This takes advantage of the generally similar nature of the geometry and internal fields over a wide variety of domain sizes so as to avoid excessively fine or coarse discretizations at maximum and minimum domain sizes.

The cases of parabolic and hyperbolic evolution equations for the internal domain are considered. The mapping shows that the true nature of parabolic equations is usually mixed parabolic/elliptic.

The evolution of the coupled system is solved by an implicit marching scheme. The discretizations in space and in time are second-order accurate. Multi-point upwinding is used to avoid an instability arising when advective terms are large.

The evolution equations are non-linear, and are solved using a nested Newton-Raphson procedure. The nesting is achieved by using successively better approximations to the true evolution equations. The matrix that arises is solved using an incomplete Cholesky factorization as a pre-conditioning method with a conjugate-gradient-like (ORTHOMIN) iteration procedure.

Improved Accuracy in Generating Forward Difference Estimates for the Solution of the Optimal Control Problem

M K Horn, Messerschmitt-Bölkow-Blohm, F.R. Germany.

In numerical solutions of the optimal control problem, the use of forward difference approximations for estimating the partial derivatives of the cost function and the boundary conditions can reduce user effort and set-up time. These advantages, however, can be off set by increased computing time if the inaccuracies arising from the perturbation size slow down the convergence rate. By restructuring the right hand sides of the ordinary differential equations (ODEs), one can essentially integrate the difference between the perturbed solution and the nominal solution to the same accuracy as that of the nominal solution. This permits the use of smaller perturbations, and hence, yields higher accuracies in the forward difference estimates. The "restructuring" of the ODEs is simplified by the use of a software package for the basic functions, so that little additional user effort is required for modeling the equations. Theory and results are presented using Runge-Kutta formulas of paired orders (4)5 and 7(8). Particular attention is paid to the treatment of time-related design parameters, e.g. initialization of braking features, run-up to full thrust, etc. Finally, it is shown that the advantage of such an approach may be finessed by restructuring the integration package itself, depending upon the accuracy desired and the word length of the computer.

Improving the Stability of Predictor-Corrector Methods by Residue Smoothing

P J van der Houwen*; B P Sommeijer, Centre for Mathematics and Computer Science, The Netherlands.

Residue smoothing is usually applied in order to accelerate the convergence of iteration processes. Here, we show that residue smoothing can also be used in order to increase the stability region of predictor-corrector methods. We shall concentrate on increasing the real stability boundary. The iteration parameters and the smoothing operators are chosen such that the stability boundary becomes as large as $c(m,q)m^2 4^q$ where m is the number of right-hand side evaluations per step, q the number of smoothing operations applied to each right-hand side evaluation, and $c(m,q)$ a slowly varying function of m and q, of magnitude 1.3 in a typical case. Numerical results show that, for a variety of linear and nonlinear parabolic equations in one and two spatial dimensions, these smoothed predictor-corrector methods are at least competitive with conventional implicit methods.

Nonlinea .ability of O.D.E. Solvers
A Iserles, University of Cambridge.

The standard Dahlquist nonlinear stability theory for numerical ODE's aims at extending the scope of the linear theory. This has led to great many important insights. However, in this talk we approach the underlying problem from the opposite point of view, elucidating phenomena that are genuinely nonlinear and that cannot be explained by the linear theory.

Our analysis focuses on the Riccati equation, both scalar and vector. We investigate the maintenance of the correct asymptotic behaviour by multistep and Runge-Kutta methods and examine the influence of various nonlinear algebraic solvers. This is being done with techniques from the theory of dynamical systems.

Some of our results will be, to say the least, surprising to the linearly minded - e.g., it is strongly advantageous to use an even number of corrector iterations in the Predictor-Corrector implementation of Forward Euler and the Trapezoidal Rule.

Order of Convergence of Quasi-Interpolation Using Radial Basis Functions
I R H Jackson, University of Cambridge.

In this paper only quasi-interpolation on a regular grid in R^n will be considered. For such a method it is necessary to have a function $\psi(x)$ defined on R^n for which

$$\int_{R^n} |\psi(x)|dx < \infty \qquad \text{and} \qquad \int_{R^n} \psi(x)dx = 1.$$

In this case the quasi-interpolant to a function f define on R^n, on a regular grid of spacing h, is

$$a_h(x) = \sum_y f(y)\psi(h^{-1}(x-y))$$

where the sum is taken over all of the mesh points of a regular grid of spacing h, one of which is at the origin.

If $\psi(.)$ has the "radial basis function" form

$$\psi(x) = \sum_{i=1}^{m} \mu_i \|x - x_i\|,$$

which is achievable when n is odd (Jackson, DAMTP 1986/NA6), it is shown that further conditions may be put on $\{\mu_i\}$ and $\{x_i\}$ that ensure that, on an integer grid in R^{2n+1}, the quasi-interpolant of any polynomial of degree at most $2n + 1$ is the polynomial itself. From this result it is deduced that, if f is sufficiently smooth, the quasi-interpolant $a_h(x)$ satisfies

$$|a_h(x) - f(x)| = O(h^{2n+2}) \quad \text{for all} \quad x \in R^{2n+1}.$$

This provides a surprising extension to the fact that linear interpolation in one dimension on a regular grid is of second order.

EPDCOL: A More .ficient PDECOL Code

P Keast*; P Muir, Dalhousie University, Canada.

The algorithm PDECOL (Algorithm 540, Trans. Math. Soft., vol. 5, pp.326-351) is a popular code among scientists who have to solve systems of non-linear partial differential equations. The code is based on a method of lines approach, with collocation in the space variables to reduce the problem to a system of ordinary differential equations. There are three principal components : the basis functions employed in the collocation; the method used to solve the system of ordinary differential equations; and the linear equation solver which handles the linear algebra. This talk will concentrate on the third component, and will report on improvements in the performance of PDECOL resulting from replacing the linear algebra modules of the code by modules which take full advantage of the special structure of the equations which arise. Savings of up to 50% in total execution time can be realised.

Galerkin/Runge-Kutta Discretizations for Parabolic Equations

S L Keeling, NASA Langley Research Centre, U.S.A.

A new class of fully discrete Galerkin/Runge-Kutta methods is constructed and analyzed for parabolic equations which are (1) semilinear, (2) linear with time dependent coefficients, and (3) quasilinear. Unlike any classical counterpart, this class offers arbitrarily high, optimal order convergence. In support of this claim, error estimates are proved, and computational results are presented. Additionally, for the problems in which the time stepping equations involve coefficient matrices changing at each time step, a preconditioned iterative technique is used to solve the linear systems only approximately. Nevertheless, the resulting algorithm is shown to preserve the optimal order convergence rate while using only the order of work required by the base scheme applied to a linear parabolic problem with time independent coefficients. Furthermore, it is noted that special Runge-Kutta methods allow computations to be performed in parallel so that the final execution time can be reduced to that of a low order method.

The Inflection Points on the Curve of Cubic-Quartic Spline Fit

Ha-Jine Kimn, Ajou University, South Korea.

Since the slope of a curve is maximum and minimum at the inflection point, it is very interesting to localize exactly the inflection point in order to know well the critical situation of the given phenomenon. Some of these phenomena are known frequently by the erroneous data with uncertainty. We have already proposed the adoption of the cubic-quartic spline fit to represent these phenomena.

We seek an algorithm for the systematic usage to obtain the inflection points on the curve constructed by the cubic-quartic spline fit.

A Paralle. .lgorithm for the General LU-Factorization

D R Kincaid*; T C Oppe, The University of Texas at Austin, U.S.A.

An algorithm for computing in parallel the general LU-factorization of a matrix is presented. As special cases, one obtains the Doolittle, Crout, and Cholesky methods. The algorithm was implemented and tested on the Cray X-MP/48.

Expansion Coefficients for Powers of some Trigonometric Functions in Series of Jacobian Elliptic Functions

A Kiper*; S Wrigge, Middle East Technical University, Turkey.

The Fourier series coefficients for the Jacobian elliptic functions and their powers had been studied and recurrence formulae had been obtained. It is also possible to obtain expansions for trigonometric functions in Jacobian elliptic functions. In this work, the expansion coefficients for $\sin^m(\pi x)$ and $\cos^m(\pi x)$ in powers of Jacobian elliptic functions, with $m \geq 1$ are studied. Four-term recurrence formula are obtained and computational aspects of these coefficients are discussed.

Integral Equation System for Turbulent Diffusion

P Kirkegaard*; L Kristensen, Riso National Laboratory, Denmark.

When describing the development of a Gaussian cloud of particles with time in a turbulent medium, a non-linear two-dimensional integral equation system of the Volterra type arises. This work discusses an iterative solution method for these equations. Semianalytical techniques are used for extraction of both the near-field and the far-field properties of the solution. Computat'onal results with the algorithm including its convergence properties are reported.

The order of B-convergence for algebraically stable Runge-Kutta methods

J F B M Kraaijevanger, University of Leiden, The Netherlands.

In [1] and [2] the concept of algebraic stability was introduced for Runge-Kutta methods. It is well known that algebraic stability is equivalent to contractivity on the class of dissipative problems. In this talk we show that algebraic stability is also equivalent to B-convergence on certain classes of strictly dissipative problems. It turns out that the order of B-convergence is generally equal to the stage order.

[1] K. Burrage and J.C. Butcher: Stability criteria for implicit Runge-Kutta methods. SIAM J. Numer. Anal. 16, 46-57 (1979).

[2] M. Crouzeix: Sur la B-stabilité des méthodes de Runge-Kutta, Numer. Math. 32, 75-82 (1979).

[3] M.N. Spijker: The relevance of algebraic stability in implicit Runge-Kutta methods. IN: Numerical treatment of differential equations, K. Strehmel (ed.), Teubner 1986, 158-164.

On the Solvabil of the System of Equations Arising in Imp t Runge-Kutta Methods

M Z Liu, University of Leiden, The Netherlands.

In this talk we present a new condition under which the system of equations arising in the application of an implicit Kunge-Kutta method to a stiff initial value problem, have unique solutions. We show that our condition is weaker than related conditions presented in [1] and [2]. It is proved that the Lobatto IIIC methods fulfil the new condition.

[1] M.Crouzeix and W.H. Hundsdorfer and M.N. Spijker: On the existence of solutions to the algebraic equations in implicit Runge-Kutta methods. BIT 23, 84-91 (1983).

[2] W.H. Hundsdorfer and M.N. Spijker: On the algebraic equations in implicit Runge-Kutta methods. Report NM-R 8413, Centre for Mathematics and Computer Science, Amsterdam (1984). To appear in SIAM J. Numer.Anal.

A Nonlinear Multigrid Algorithm and Boundary-Fitted Coordinates for the Solution of a Two-Dimensional Flow in a Branching Channel

G Lonsdale*; J S Bramley; D M Sloan, University of Bradford.

A recent paper by Bramley and Sloan (Computers and Fluids (1987) describes a numerical solution for two-dimensional flow of a viscous, incompressible fluid in a branching channel. A grid generation algorithm was used to map the solution region onto a rectangle and an upwind finite difference scheme was then used to solve the Navier-Stokes equations in terms of stream function and vorticity. Here we extend the earlier work by describing an efficient solution of the problem using a nonlinear multigrid algorithm. Of particular interest is the treatment of the boundary conditions in a manner which does not destroy the interior smoothness in the neighbourhood of the boundary.

A Block-by-Block Method for Volterra Delay Integro-Differential Equations with Weakly-Singular Kernel Combined with Product Integration on Nonuniform Meshes

A Makroglou, Ministry of Agriculture, Greece.

The solution of weakly-singular Volterra integro-differential equations has in general end-point singularities at the left end-point of the interval of integration. Block-by-block implicit Runge-Kutta methods applied to such equations on uniform meshes give poor convergence rates. In this paper these methods are generalized so that they can also be used with nonuniform mesh and are applied to weakly singular Volterra delay integro-differential equations with constant and/or variable state independent delay. The kernel is assumed nonlinear and thus Gauss integration methods for the evaluation of the resulting integrals. The paper is a generalization of Makroglou (8,10,11,12).

Localised and Chaotic Patterns in a two phase flow

V S Manoranjan, University of Surrey.

A counter-current two phase flow of much interest is gas-liquid annular flow in vertical cylinders. A mathematical model which captures the essential features of this physical problem is studied in order to understand the various localised and chaotic patterns observed in the 'flooding' region.

Improving Gauss-Seidel Iterations by Means of Partial Elimination

J P Milaszewicz, Ciudad Universitaria, Argentina.

If we consider the linear system $Ax = b$, with A an irreducible M-matrix, the elimination of some unknowns yields better convergence rate for the corresponding Jacobi iterations, when compared with those for the original system. This is not always the case if Gauss-Seidel iterations are compared. We give sufficient conditions on the nodes to be eliminated that yield improvement on Gauss-Seidel iterations. Such conditions are always satisfied when A is symmetric.

Periodic Solutions of Non Linear Partial Difference Equations in Reaction-diffusion

A R Mitchell and P John-Charles, University of Dundee.

The non linear reaction diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(u \frac{\partial u}{\partial x}\right) + u(1 - u)$$

and discretisations of it in space and time model many problems in mathematical biology. It is shown by numerical experimentation that stable periodic travelling wave solutions exist beyond the von Neumann linearised stability limit, even when the grid sizes in space and time are small.

A Modified Moving Finite Element Method for Moving Boundary Problems

R O Moody, University of Reading.

A modified Moving Finite Element Method is described and applied to three standard one-dimensional moving boundary problems: one- and two-phase Stefan and the Crank-Gupta oxygen diffusion with absorption. Very favourable results are obtained for both the dependent variable and the boundary/interface position, using a small number of elements.

Quadrature Formulae for Cauchy Principal Value Integrals of Oscillatory Kind

G E Okecha, University of Calabar, Nigeria.

The problem considered is that of evaluating numerically an integral of the form $\int_{-1}^{1} e^{iwx} f(x)\,dx$, where f has one simple pole in the interval $[-1,1]$. Modified forms of the Lagrangian interpolation formula, taking account of the simple pole are obtained, and form the bases for the numerical quadrature rules obtained. Further modification to deal with the case when an abscissa in the interpolation formula is coincident with the pole is also considered. An error bound is provided and some numerical examples are given to illustrate the formulae developed.

On Certain Minimal Polynomials Related to the Iterative Solution of Linear Equations

G Opfer, University of Hamburg, F.R. Germany.

The iteration scheme $x_{j+1} = x_j - \alpha_j(Ax_j - b)$, $i = 1,2,\ldots$, for solving the (real or complex) linear $N \times N$ system $Ax = b$ is particularly well suited for parallel computation, since all components of x_{j+1} can be computed independently and therefore simultaneously.

We assume that a set S which contain the spectrum $\sigma(A)$ of A is known. The above iteration converges if the parameters α_j are chosen such that $\|p\|_\infty < 1$, where $p(z) = \Pi_{j=1}^{n} (1 - \alpha_j z)$, $\alpha_{kn+j} = \alpha_j$, $j=1,2,\ldots,n$ for any $k \in \mathbb{N}$ and $n \in \mathbb{N}$ fixed (cyclic iteration with cycle length n). Therefore the knowledge of the minimal polynomials which minimise $\|\cdot\|_\infty$ within all $p \in \Pi_n$ with $p(0) = 1$ is essential for finding the above mentioned α's. In all cases the maximum norm $\|\cdot\|_\infty$ has to be computed on S.

For $n = 1$ and arbitrary sets S the problem has been solved by F. SCHOBER and the lecturer (LAA 58(1984),343-361). We shall report on results mainly for $n=2$ and rectangular inclusion sets S. These sets are particularly well suited for eigenvalue inclusions due to a theorem by BENDIXSON.

A New Approach to Sameh's Parallel Eigenvalue Algorithm

M H C Paardekooper, Tilburg University, The Netherlands.

This paper presents an improved version of Sameh's parallel eigenvalue algorithm. It constructs a sequence $\{A_k\}$ with $A_{k+1}=S_k^{-1}A_kS_k$, $k \in \mathbb{N}$ where the normreducing transformation matrix S_k is a direct sum of unimodular two-dimensional shears. These Jacobi-like shear transforms can be carried out concurrently. An appropriate choice of the non-trivial elements of S_k together with a well-chosen pivot-strategy provides that $\{A_k\}$ tends to normality: $A_kA_k^T-A_k^TA_k \to 0$ $(k\to\infty)$. As a consequence of the invariance of the Frobenius matrix norm under orthogonal transformation the norm-reduction should be discussed in theoretical terms that are invariant under these transformations. In our modification of Sameh's algorithm the problem formulation with so-called Euclidean parameters improves and simplifies the procedure and the formulae in the related minimization problem.

Different aspects of the method (global convergence, speed of convergence) and its implementation (communication, storage strategy) are discussed.

Gaussian Quadrature Formulas for Splines with an Application to Integral Equations

L Pretorius*; D P Laurie; D Eyre, NRIMS, South Africa.

The existence of Gaussian quadrature formulas for splines was shown, for example, by [Karlin and Studden, 1966] and also [Micchelli and Pinkus, 1977]. However, the computational construction of these formulas received little attention in the literature. This may be a consequence of the fact that most methods for constructing the classical Gaussian quadrature formulas rely heavily on the powerful theory of orthogonal polynomials and therefore do not apply in the case of splines. In this presentation we discuss the construction of Gaussian quadrature formulas for splines and then successfully apply them to integral equations.

S. Karlin and W. J. Studden, 1966. Tchebycheff systems: with applications in analysis and statistics. New York: Interscience Publishers, a division of John Wiley.

C. A. Micchelli and A. Pinkus, 1977. Moment theory for weak Chebychev systems with applications to monosplines, quadrature formulae and best one-sided L^1-approximations by spline functions with fixed knots. SIAM Journal of Mathematical Analysis, 8, 206-230.

Solving Nonline_'Equality Constrained Optimisation Problems Áing the Truncated Newton Method with Automatic Differentiation

R C Price, Hatfield Polytechnic.

In this paper we are concerned with nonlinear equality constrained optimisation problems. The minimum of the Di Pillo-Grippo penalty function occurs at the minimum of the corresponding constrained problem. In previous work we have applied the truncated Newton Method to unconstrained problems [1], where the required derivatives have been obtained by automatic differentiation [2]. In this paper we extend these ideas and apply them to the Di Pillo-Grippo penalty function. All the derivatives are obtained in such a way that the hessians of each constraint are stored one at a time and not simultaneously, thus making the method low on storage requirements.

Encouraging results have been obtained when the method has been applied to a series of test problems.

[1] Numerical experience with the truncated Newton method. Technical Report No. 169, NOC, The Hatfield Polytechnic. (To appear in *Journal of Optimisation Theory and Applications*).

[2] The truncated Newton method for sparse unconstrained optimisation using automatic differentiation. Technical Report No.170, NOC, The Hatfield Polytechnic. (To appear in Journal of Optimisation Theory and Applications).

An Alternative to Chan's Deflation for Bordered Systems

J D Pryce, University of Bristol.

Linear systems like

$$M\begin{bmatrix} x \\ y \end{bmatrix} \equiv \begin{bmatrix} A & b \\ c & d \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

frequently occur in numerical continuation and other contexts. Here A is $n \times n$, G is $n \times 1$, c is $1 \times n$ and d is a scalar, and A is structured (sparse, banded, etc.) while the 'border' b, c and d is usually full. The complete $(n+1) \times (n+1)$ matrix M is assumed to be well conditioned but A may be arbitrarily near to singularity. However, for efficiency's sake we wish to use a solver for linear systems of the structure of A, as a black box. How to do this and come out with accurate answers even when A is ill-conditioned?

The talk will present an alternative to the frequently used deflation method of T. F. Chan. The new method, due to W. Govaerts and the speaker, is simpler to program and in a large number of tests on moderate-sized matrices has not been found to fail.

Work on the case of borders of width k, $1 < k << n$, will also be mentioned.

A Numeri , Stratified Model for Hurricane Generated rrents

K K Puri*; C Cooper, University of Maine, U.S.A.

A multi-layer model is considered to study hurricane generated currents in an ocean environment. It consists of four layers. The upper most mixed layer admits the presence of a free surface and hence of the atmospheric pressure gradients. Its interaction with the lower layer permits its thickening as a result of entrainment due to the shear instabilities.

The time dependent equations, appropriate to the four layers which take into account the Coriolis effect are solved numerically using an explicit finite difference scheme. The results are compared with existing current models which this model subsumes. Also, barotropic and baroclinic responses are sought, to the presence of hurricanes Fredricks and Allen.

A Spline Approximation Method for Solving System of O.D.E.

I Refat, Ministry of Education, Kuwait.

In this paper we consider the system of second order ordinary differential equations with initial conditions. We constructed a spline function, which is not necessarily polynomial spline, approximating the solution of this problem and giving optimal error bounds.

Accuracy of Difference Schemes for Solving the Wave Equation

R Renaut, Arizona State University, U.S.A.

Time stepping schemes for the solution of the wave equation are analysed. It is demonstrated that the determination of stability and order of accuracy properties of these schemes can be posed as a rational approximation problem. Applying order star techniques a bound on accuracy is derived. Further, all of the schemes attaining this bound are stable. Similar analysis leads to a bound on accuracy of full discretisations of the wave equation. The explicit methods are stable for Courant numbers less than one.

Choices in Contractivity Theory of One-Leg and Multistep Methods

J Sand, University of Copenhagen, Denmark.

Contractivity theory has in the past been used as a rather powerful tool for establishing stability results for the solution of ordinary differential equations (ODE's). The applicability of the tool is, however, strongly dependent on three choices, which have to be made, viz.

- The class of ODE's to be considered.
- The class of methods to be applied.
- The type of norm in which contractivity is to hold.

Restricting ourselves to the classes of one-leg and linear multistep methods, we shall review some of the choices which have been examined in the past and suggest alternatives which in certain cases lead to less pessimistic results.

Stability Phenomena Arising in the Numerical Study of a Fluidized Bed

J M Sanz-Serna*; L Abia, Universidad de Valladolid, Spain.

When numerically studying an evolutionary partial differential equation modelling a fluidized bed, I. Christie and G. Ganser found a number of remarkable stability phenomena (see their contribution to this conference). Crank-Nicolson /implicit midpoint time discretizations of reasonable finite difference or Galerkin space discretizations turned out to be unstable, while schemes based on the backward difference formulae behaved in a stable manner only if the time step was chosen to be large relative to the mesh size in space.

In the present contribution we analyze in detail these phenomena and suggest new schemes which do not suffer from stability problems. The nonlinear stability and convergence of the new methods is studied within a framework developed by J. C. Lopez-Marcos and one of the present authors (J.M.S.).

Best Parametric Interpolation by Cubic Splines in $\mathbb{R}^d$

K Scherer, University of Bonn, W. Germany.

The problem of finding a curve by passing through prescribed points in $\mathbb{R}^d$ is considered such that the kinetic energy of a particle moving along this curve is minimized. Since the moment of passing is free (within a given time) this results in a nonlinear problem. The uniqueness of its solution is proved by showing that it is equivalent to a convex programming problem. Also the shape preserving properties of the solution are discussed.

High Wave Modulations in Numerical Solutions of the Korteweg-De Vries and Modified Korteweg-De Vries Equations

S W Schoombie, University of the Orange Free State, South Africa.

The results of numerical experiments are presented, showing a solitary sawtoothed wave packet emerging from rectangular pulse initial data. In the case of the MKdV - equation an analysis shows such wave packets to have envelopes satisfying a different MKdV - equation. Thus sawtoothed envelope solitons become a possibility. These phenomena are due to the nature of the space discretization used, which is a central difference scheme. A multiple scales analysis shows that modulated sawtoothed waves of small amplitude satisfy a linear dispersive difference equation.

ERNY - A[illegible]plicit Runge-Kutta Nystrom Integrator for [illegible]nd Order Initial Va[illegible]ue Problems

P W Sharp*; J M Fine, University of Toronto, Canada.

In this paper we discuss an integrator we have developed for second order initial value problems for the form $y'' = f(x,y)$, $y(x_0) = y_0$, $y'(x_0) = y'_0$. The integration is performed using an explicit (4,5) Runge-Kutta Nystrom pair with error control on y and y'. Local extrapolation is employed and y and y' are estimated at the output points using interpolants that do not require extra derivative evaluations. We begin by summarizing properties of the (4,5) pair and the interpolants. Following this the performance of the integrator is illustrated for several test problems on a scalar machine. Finally we discuss how the integrator can be modified to take advantage of the vectorizing and multitasking capabilities of a CRAY X-MP/2.

Solving Linear Partial Differential Equations by Exponential Splitting (I)

Qin Sheng, University of Cambridge.

Let $A_1, A_2, \ldots, A_N$ be square matrices which do not commute. We consider approximations to the matrix exponential $M(t) = \exp\{t(A_1+A_2+\ldots A_N)\}$ of the form $\sum_{k=1}^{k} \gamma_k E_k$, where each γ_k is a multiplying factor, and each E_k is a product of terms, each term having the form $\exp\{\alpha t A_n\}$ for some $\alpha > 0$ and $1 \le n \le N$. This form is relevant to semi-discretization methods for linear partial differential equation problems, and it produces systems which are easy to solve. The accuracy and stability of this splitting approximation are studied. It is shown that, even if the number of terms and the number of values of k are chosen to be large, the highest order of a stable approximation is two. Numerical examples are given.

Upwinding on Triangular Elements

S Sigurdsson, University of Iceland.

Upwinding techniques for one-dimensional, steady-state, convective transport equations in the framework of Petrov-Galerkin methods have been studied extensively by many authors. However, the question of extending these techniques to two-dimensional problems, in particular in the case of irregular triangular finite elements seems as yet not to have been fully resolved. We present different viewpoints of this question with special emphasis on linear basis functions and describe techniques that have been used for solving groundwater contamination problems.

A Locally Mass Conserving, Quadratic Velocity, Linear Pressure Element for Incompressible Flow

D J Silvester, UMIST.

One of the most popular triangular elements for 2D incompressible flow problems is the continuous quadratic velocity, continuous linear pressure element. The principal attraction of the element is its uniform stability coupled with its cost-effectiveness. Despite the element's general acceptability, serious doubts concerning its performance have also been expressed. In particular, the inherent lack of continuity concomitant with a continuous pressure approximation is known to give rise to non-physical solutions if the flow problem is sufficiently 'difficult'. For example, poor results using the element to model recirculating isothermal flows and strongly coupled thermal flows have been presented previously. A less well-known class of problems which also demonstrate this behaviour is that of non-Newtonian flow.

To improve the approximation of such flows a 'hybrid' element having two superposed pressure fields has been analysed and tested numerically. In particular, supplementing the basic pressure field with a piecewise constant pressure field has been shown to lead to an improved mixed approximation which is still uniformly stable. By way of illustration, the performance of the modified element is contrasted with that of the conventional element for a rudimentary non-Newtonian swirling flow.

Piecewise Polynomials and Integrodifferential Equations

I M Snyman*; S A Sofianos, University of South Africa.

The integrodifferential equation derived in the framework of the Hyperspherical Harmonics method to describe the bound state of a three-boson system in configuration space, has been solved using B-splines. The equation includes the strong effects of the hypercentral part of the two-body potential and has apparent singularities as well as δ-function type behaviour in the asymptotic region. B-splines proved to be particularly suitable to handle these difficulties. The Galerkin method is used together with soft and hard core two-body interactions to obtain upper and lower bounds for the binding energy of the system. Various numerical aspects of the problem such as stability of the method, choice of mesh points and the order of the B-splines are discussed.

A Generalisation of Godunov's Method via Randomly Sampled Intercell Fluxes

E F Toro, Cranfield Institute of Technology.

A large variety of modern computational techniques for quasi-linear hyperbolic equations make use of the solution of the Riemann problem.

Here, yet another method is presented in which to update the solution at cell i a leap-frog finite difference scheme is used, i.e.

$$U_i^{n+1} = U_i^n - \frac{\Delta T}{\Delta x}\left(F_{i+\frac{1}{2}}^{n+\frac{1}{2}} - F_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right)$$

where intercell fluxes $F_{i+\frac{1}{2}}^{n+\frac{1}{2}}$ are evaluated at the solution of the Riemann problem $RP(i, i+1)$ at a randomly given point $P_i = (x, t_{n+\frac{1}{2}})$ with $x = (i - \frac{1}{2})\Delta x + \theta^n \Delta x$. Here θ^n is a quasi-random number in the interval $[-\frac{1}{2}T, \frac{1}{2}T]$ and T is an interval-length sampling function varying between $T = 0$ and $T = 1$. Every value of T in $[0,1]$ gives a difference scheme; in particular $T = 0$ reproduces Godunov's first order method, $T = 1$ gives a second order method that can be interpreted as a random Lax-Wendroff Method.

Suitable construction of the function T leads to a method that ranges through the family of schemes described above giving higher accuracy than Godunov's Method and which is also monotone.

Applications to the Euler equations in one and two dimensions are made.

On the Convergence of the Product Approximation in Semilinear Problems

Y Tourigny, University of Dundee.

By means of a concrete example, we will first explain what the so-called product approximation in the finite-element method consists of. We will then review the existing convergence theory for this technique. At the moment, the theory covers such problems as: nonlinear Klein-Gordon equations, nonlinear Schrödinger equations, nonlinear parabolic equations and semilinear two-point boundary value problems.

Is Gaussian Elimination Stable?

L N Trefethen*; R S Schreiber, MIT, U.S.A.

Wilkinson showed that Gaussian elimination with partial pivoting is stable so long as the "growth factor" is not too large. But he also showed that in the worst case it is too large - 2^{n-1} for a matrix of dimension n. Thus Gaussian elimination is unstable in the worst case.

Why then does this tried-and-true algorithm work so well in practice? Some people have proposed that the matrices that arise in practical problems must be exceptionally well-behaved. In this talk we show that there is no need for that hypothesis. In fact, Gaussian elimination is stable on average, and the average-case growth factor is no worse than n. We support these claims with empirical evidence and the beginnings of a theoretical explanation.

Some Stability Results for the Hopscotch Difference Method when Applied to Convection-Diffusion Equations

J G Verwer, Centre for Mathematics and Computer Science, The Netherlands.

The hopscotch method is a time stepping scheme applicable to wide classes of spatially discretized, multispace dimensional, time-dependent partial differential equations. In this contribution attention is focussed on the simple odd-even hopscotch method. Our aim is to present some interesting, linear stability results of this method for convection-diffusion equations, where the space discretization is carried out by standard symmetrical and/or one-sided finite differences. We present two sorts of results. The first result is concerned with von Neumann stability in the multi-dimensional case. Here we derive expressions for the critical time step and show that in certain cases an increase of diffusion may render the process unstable, an observation which is in clear contrast to the common practice. This strange phenomenon can occur only in the higher dimensional case. The second result is concerned with the spectral condition, but only in one space dimension. We derive the critical time step values and conclude, in accordance with known results for the explicit Euler rule, that the spectral condition is misleading in the sense that it does not prevent large error growth.

A Type-Insensitive ODE Solver

K C Wade ; C W Richards ; M G Everett , Thames Polytechnic, London.

A variety of efficient integration algorithms, in the form of subroutine libraries, are available for the solution of initial value problems in ODE's. However it is left to users to select the most appropriate algorithm for their problem. Frequently inexperienced users select unsuitable algorithms such as attempting to integrate stiff systems using explicit Runge-Kutta methods. The situation is further complicated when, as often happens in engineering problems, the characteristics of the equations change during the integration range.

This paper describes a numerical code based on Runge-Kutta methods that assesses the characteristics of the equation throughout the integration range and automatically selects the most appropriate integration method. A total of three explicit Runge-Kutta and four implicit Runge-Kutta methods are available giving a variable step, variable order algorithm. The strategy employed in selecting order and in switching beteen explicit and implicit methods is described. To ensure that the switching strategies are efficient an embedding technique is employed, which requires no additional function evaluations.

Numerical results are presented which demonstrate the effectiveness of the switching technique and overall efficiency of the code.

Global Preconditioning for Galerkin Finite Element Equations Using Element-by-Element Analysis

A J Wathen, University of Bristol.

It is traditional in Finite Element calculations to assemble information from the individual elements into large global matrix systems, then to solve using elimination methods. The matrix is usually large and is generally assumed to be banded about the diagonal or to have some sparsity structure. Such a general approach ignores the specific structure which is due to the construction (assemblage) of the matrix itself. In this paper we show how properties of the matrix which are useful in the solution process can be derived simply from observations regarding the assemblage of the global matrix from individual element matrices. Specifically we show how to derive eigenvalue bounds for symmetric finite element coefficient matrices with simple preconditioners which are formed also by an assembly process. These bounds on the eigenvalues of the preconditioned global matrix are derived element-by-element and have been used by the author to guarantee rapid convergence of the Preconditioned Conjugate Gradient Method for the solution of finite element equations. We give results for diagonal and tridiagonal preconditioning of Galerkin mass and stiffness matrices for many common types of element in 1- 2- and 3-dimensions as well as an example of the wider use of the technique. It will also be shown how this work explains some of the success of Hughes' element-by-element algorithm for elliptic problems (Hughes, T.J.R., Levit, I. and Winget, J., Comput. Meths. Appl. Mech. Engng. 36, 241-254, 1983).

The Smallest Perturbation of a Submatrix which Lowers the Rank of a Matrix

G. A Watson, University of Dundee.

The problem is considered of determining the smallest perturbation of a submatrix of a partitioned rectangular matrix which achieves for that matrix a given lower rank. For different classes of matrix norms, it is shown how the solution of the problem can be obtained through an equivalent, often simpler problem.

The Eigenvalues of Spectral Differentiation Matrices

J A C Weideman*; L N Trefethen, MIT, U.S.A.

Spectral methods for partial differential equations are based upon the approximation of space derivatives by global trigonometric or polynomial interpolation followed by differentiation of the interpolant. This process is equivalent to the multiplication of the data vector by a matrix D. The eigenvalues of D are of fundamental importance to the stability and other numerical properties of such methods. This talk surveys old and new results on the distribution of these eigenvalues for fundamental spectral problems involving first- or second-order differentiation in equispaced or Chebyshev points.

An Algorithm for Minimizing a Quadratic Function with Quadratic Constraints
Y Yuan, University of Cambridge.

We study the problem of minimizing a general quadratic function with special quadratic constraints. This problem is a sub-problem in some trust region algorithms for general nonlinear optimization. An algorithm is presented.

The Rate of Convergence of Sliding Block Jacobi Schemes
Yong Li; W Ferguson*, Southern Methodist University, U.S.A.

The sliding block Jacobi schemesconsidered in this paper are q-line block Jacobi schemes in which the last r-lines of one block are overlapped with the first r-lines of the next block. Analytic formulas for the spectral radius of these sliding block Jacobi schemes are presented for a class of model problems which includes the classical Poisson equation on a rectangle. Well known formulas relate the spectral radius of the Jacobi scheme to the rate of convergence of associated SOR and CG schemes. Sliding block Jacobi schemes may form the basis of robust and efficient iterative schemes for solving elliptic partial differential equations on parallel computers because their rate of convergence increases rapidly with increasing values of q and r.

Iterative Methods for Nonlinear Operator Equations of Monotone Type
You Zhaoyong*; Xu Zongben, Xi'an Jiaotong University, P.R. China.

Many problems arising naturally in the field of differential equations, integral equations, variational methods and optimizations involve the solution of equations associated with nonlinear operators of monotone type. In this paper, we systematically develop iterative methods for solving such different type of monotone operator equations, which includes:

- Relaxation iterative processes for strongly monotone operators
- A second order difference regularization approach to maximal monotone operators
- A class of iterative method with finite termination property
- Ergodic convergence of Ishikawa's method for general monotone operators.

<u>Upper and Lower Bounds to Eigenvalues of Eigenvalue Problems with Partial Differential Equations</u>

S Zimmermann, Technische Universität Clausthal, Germany.

This paper deals with eigenvalue problems $M\phi = \lambda N\phi$ ($\lambda \in \mathbb{R}$ eigenvalue, $\phi \in H$ eigenvector), where M, N are linear symmetric operators in a Hilbert space H. Accurate upper bounds to eigenvalues can often be obtained by applying the Rayleigh-Ritz method. For calculating corresponding lower bounds one can sometimes employ the Lehmann-Maehly method, which contains the well-known Temple formula as a special case. A generalization of this method has been proposed by Goerisch recently, it possesses a much larger range of application. The convergence of both Lehmann and Goerisch's bounds is studied. Numerical results are given for the plate problems

$$\Delta^2\phi = -\lambda\Delta\phi \quad \text{in } \Omega, \quad \phi = \frac{\partial\phi}{\partial n} = 0 \quad \text{on } \partial\Omega \qquad \text{(buckling)},$$

$$\Delta^2\phi = \lambda\phi \quad \text{in } \Omega, \quad \phi = \frac{\partial\phi}{\partial n} = 0 \quad \text{on } \partial\Omega \qquad \text{(vibration)}.$$